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PREDICTION OF OZONE FROM METEOROLOGICAL PARAMETERS FOR USE IN GLOSS AND UV INDEX FORECASTING

by

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February 1994

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1. INTRODUCTION

NESDIS (National Environmental Satellite Data Information Service) data, consisting of cloud-cleared brightness temperatures, satellite information, and satellite derived quantities are used in the GLOSS (Global Satellite Sounding System) retrieval scheme [*Gadd et al*, 1994].

The cloud-cleared brightness temperatures along with a global model background (6 hour forecast) output by the operational numerical weather prediction model [*Cullen*, 1993], provide the input to a GLOSS retrieval. One of the satellite derived quantities is total column ozone [*Chesters and Neuendorffer*, 1991]. This is required by the forward model [*Eyre*, 1991], in deriving background brightness temperatures from the model background profile. Ozone can have a significant influence when deriving background brightness temperatures for some of the HIRS (High-resolution Infrared Radiation Sounder) temperature sounding channels.

2. THE NEED FOR SUBSTITUTE OZONE VALUES

NESDIS ozone values can be absent from the data. This occurs mainly in cloudy fields of view (*figure 1a*), but also in some clear fields of view (*figure 1b*). Figure 1a shows the missing ozone values for cloudy fields of view for a single day in January 1994. As there are fewer missing ozone values for clear fields of view, figure 1b shows the missing values for a 2 week period in January 1994 to emphasise the areas of interest. The missing ozone values in clear fields of view occur most often over ice or high ground (e.g. Greenland and Antarctica), but there are also missing values in lines near 30°N and 60°N, and to a lesser extent near 30°S and 60°S.

Originally in GLOSS processing, for the cases when the NESDIS ozone value was missing, a substitute value of 347 Dobson units was used. This is a climatological value for the local (UK) area. It is necessary to provide substitute ozone values which are globally more representative. Other requirements are that the substitute values are easily calculated and that a value can always be provided where a retrieval is to be performed.

Ozone amount varies enormously over the globe. An approximate range is 100 - 500 Dobson units for individual HIRS fields of view. There is also quite a large

seasonal variation which needs to be taken into account. A plot of 10 degree latitude/longitude boxed means of NESDIS ozone observations for a day in January 1994 is shown in *figure 2a* and for a day in July 1993 in *figure 2b*.

In the forward model RTTOV [*Eyre, 1991*], ozone is used in the calculation for HIRS channels 1-7. *Tables 1a,1b,1c* show how background brightness temperatures in these channels vary with ozone amount. The tables show the channel number, the change in temperature for each ozone Dobson unit change, and the change in ozone needed to alter the background brightness temperature by 0.1 deg K. *Table 1a* is for a typical polar temperature profile, *table 1b* for a mid-latitude profile and *table 1c* for a tropical profile.

Polar profile		
Channel no.	*dT(K) for 1 Du change*	*Du/0.1 K*
HIRS-1	0.00009	1100
HIRS-2	0.00014	714
HIRS-3	0.00001	10000
HIRS-4	-0.00082	-122
HIRS-5	-0.00299	-33
HIRS-6	-0.00307	-33
HIRS-7	-0.00244	-41

Table 1a. The relationship between ozone and GLOSS background brightness temperatures for HIRS 1-7 for a polar profile

Mid-latitude profile		
Channel no.	*dT(K) for 1 Du change*	*Du/0.1 K*
HIRS-1	0.00010	1000
HIRS-2	0.00019	526
HIRS-3	-0.00010	-1000
HIRS-4	-0.00153	-65
HIRS-5	-0.00457	-22
HIRS-6	-0.00445	-23
HIRS-7	-0.00334	-30

Table 1b. The relationship between ozone and GLOSS background brightness temperatures for HIRS 1-7 for a mid-latitude profile

Tropical profile		
Channel no.	*dT(K) for 1 Du change*	*Du/0.1 K*
HIRS-1	0.00012	833
HIRS-2	0.00023	435
HIRS-3	-0.00037	-270
HIRS-4	-0.00244	-41
HIRS-5	-0.00614	-16
HIRS-6	-0.00568	-18
HIRS-7	-0.00407	-25

Table 1c. The relationship between ozone and GLOSS background brightness temperatures for HIRS 1-7 for a tropical profile

The need for improved ozone substitute values is illustrated by the effect of using a default value of 347 Dobson units in the tropics, where it is possible for the ozone to drop below 200 Du. This would mean a substitute value for the ozone which is 150 Du too high, producing an error in the background brightness temperature for HIRS-5 of almost a degree. In GLOSS retrievals, for non-clear fields of view, HIRS channels 1-3 are the only HIRS channels used. As these are not so sensitive to changes in ozone quantity (see *tables 1a,1b,1c*), the need for an accurate ozone replacement is really only important for clear fields of view.

3. THE OZONE REGRESSION (FOR GLOSS)

As there are only a few substitute ozone values required, the most accurate estimation would be to perform a horizontal interpolation from neighbouring ozone values. This is not straightforward, however, because the data is not received in a conveniently ordered form. For the purposes of GLOSS it was therefore decided to produce an ozone value based on a regression on a single stratospheric temperature. Global correlations between ozone and model background temperatures above 200hPa were produced. 70hPa temperature was chosen to be the predictor.

$$O_{pred} = a_0 + a_1 T_{70hPa} \tag{1}$$

where O_{pred} is the regression predicted ozone value, in Dobson units, a_0 and a_1 are the regression coefficients and T_{70hPa} is the 70hPa background temperature, in degrees Kelvin.

NESDIS ozone, and 70hPa model temperatures for an approximate 10 day long period are used in the regression. Data selection involves using those fields of view over the sea which are classed non-cloudy by NESDIS. The latter restriction was imposed to eliminate as far as possible all fields of view likely to contain cirrus clouds, since their anomalous emissivity can interact with the procedure used to remove the effect of clouds from the data so as to introduce errors in the derived ozone. To provide a more balanced global representation, latitude banding was performed for the bands 90°S — 30°S, 30°S — 30°N, 30°N — 90°N, producing near equal amounts of observations in each of these bands. The regression performed was a simple regression, described in BMDP (Biomedical Computer Programs) software BMDP1R. The ozone regression coefficients are updated monthly, with new coefficients being introduced operationally early in each month, based on statistics from the previous month.

3.1 RESULTS

So far, 6 sets of regression statistics have been produced and used operationally in GLOSS. The data periods, and regression values are shown in *table 2.*

The 6 sets of values show significant differences. Looking at sets 1 through to 4, it can be seen that predicted ozone becomes more sensitive to changes in the 70hPa background temperature field. Sets 5 and 6 show the reverse affect. This seasonal variation confirms the need for regular updates of the values for operational use.

Regression statistics			
Data period	a_0	a_1	
11/07/93 - 20/07/93	-345.25195	3.0452	set 1
03/08/93 - 17/08/93	-421.92773	3.4226	set 2
06/09/93 - 18/09/93	-569.28369	4.1125	set 3
06/10/93 - 17/10/93	-656.55298	4.5342	set 4
08/11/93 - 29/11/93	-501.88721	3.7900	set 5
04/01/94 - 15/01/94	-449.01587	3.5609	set 6

Table 2. Regression statistics introduced operationally in GLOSS

To test the ozone regression, a predicted ozone value was produced for each NESDIS field of view using equation 1 and compared to the NESDIS ozone value, and the previously used constant value of 347 Dobson units. The regression was performed in clear and non-clear fields of view, but only over a sea surface. The regression was not performed when there was missing NESDIS ozone (no comparison can be done) or when the 70hPa background temperature was missing (the retrieval wouldn't be performed anyway).

Ozone regression testing				
		30°N - 90°N	*30°S - 30°N*	*90°S - 30°S*
1	NESDIS ozone mean	328.86	251.42	287.75
2	NESDIS ozone stan dev	49.19	19.75	26.56
3	Predicted ozone mean	296.42	257.14	317.47
4	Predicted ozone stan dev	23.00	10.61	29.10
5	Default ozone mean	347.00	347.00	347.00
6	Default ozone stan dev	0.00	0.00	0.00
7	Predicted - NESDIS ozone mean	-32.44	5.72	29.72
8	Predicted - NESDIS ozone stan dev	38.37	14.34	16.65
9	Default - NESDIS ozone mean	18.14	95.58	59.25
10	Default - NESDIS ozone stan dev	49.19	19.75	26.56
11	Max (predicted - NESDIS) diff	161.56	91.59	114.36
12	Max (default - NESDIS) diff	168.00	190.00	150.00
13	No. predicted - NESDIS diffs > 30 Du	1927	1221	5852
14	No. default - NESDIS diffs > 30 Du	2759	20324	10300
15	No. NESDIS obs used	4183	20504	12637

Table 3. Ozone regression testing (for GLOSS)

Table 3. shows results using set 6 regression coefficients for the prediction, tested on an independent 24 hour period of GLOSS data for 19/01/94 21Z – 20/01/94 21Z. Results are shown for three latitude bands. For rows 11-14, the differences are absolute differences and default ozone = 347 Du.

The maximum (predicted - NESDIS) ozone difference (row 11) is less than the maximum (default - NESDIS) ozone difference (row 12), and the number of predicted - NESDIS ozone differences greater than 30 Dobson units (row 13) is less than the number of default - NESDIS ozone differences greater than 30 Dobson units (row 14) in in all 3 latitude bands. It can also be seen that the Predicted - NESDIS standard deviation (row 8) is less than the Default - NESDIS standard deviation (row 10) in all latitude bands. A plot of predicted - NESDIS ozone (over land and sea) is shown in *figure 3a*, and a plot of default - NESDIS ozone (over land and sea) is shown in *figure 3b*. Histograms of Global differences are shown in *figures 4a,4b*.

4. THE OZONE REGRESSION (FOR UV FORECASTING)

An estimate of total column ozone is required for ultra violet index forecasting. Regression coefficients are applied to forecast fields to produce an ozone forecast. Although it is acceptable for use in GLOSS, the ozone regression described in section 3 is very crude. This section describes a regression, which uses more than just a single stratospheric temperature (70hPa) to predict total ozone amount. A direct comparison between the two methods is not outlined in this report, due to the fact that the ozone regression for GLOSS has globally calculated coefficients and the regression for UV forecasting has limited area calculated coefficients. Regression coefficients, method as described in this section, have, however, been produced from and tested on global data, and seen to be a significant improvement on the regression coefficients described in section 3.

After correlation and step-wise regression studies, It was decided to use three predictors in this ozone regression. The predictors used were 1000-250hPa thickness, 150hPa background temperature and 30hPa background temperature. These quantities represent the ozone relation with tropopause height and with lower and upper stratospheric temperatures. As with the regression in section 3, data selection involves using clear fields of view over the sea. The regression is described in BMDP software BMDP1R.

$$O_{pred} = a_0 + a_1 Th_{1000-250hPa} + a_2 T_{150hPa} + a_3 T_{30hPa} \qquad (2)$$

O_{pred} is the regression predicted ozone value, in Dobson units.

$Th_{1000-250hPa}$ is the 1000-250hPa thickness, in metres.

T_{150hPa} is the 150hPa background temperature, in degrees Kelvin.

T_{30hPa} is the 30hPa background temperature, in degrees Kelvin.

a_0, a_1, a_2, a_3 are the regression coefficients.

4.1 RESULTS

At the time of writing this report, 7 sets of regression coefficients have been produced. The data periods (approximately the last week in each month) and re-

gression values are shown in *table 4*. The regression values have been produced for data in the limited area 15°N — 75°N, 60°W — 60°E, again using those fields of view over the sea and classed non-cloudy by NESDIS. The regression is intended to be used for a similar area in the UV forecasting.

Regression statistics					
Data period	a_0	a_1	a_2	a_3	
June 93	1690.55933	-0.1132	1.8489	-2.6210	set 1
July 93	1573.28784	-0.0965	1.8155	-2.9009	set 2
August 93	408.04077	-0.0381	1.7062	-0.3321	set 3
September 93	-713.97900	0.0055	2.7374	1.6604	set 4
October 93	72.57275	-0.0562	1.2228	2.5059	set 5
November 93	98.51929	-0.0725	2.4145	2.0349	set 6
December 93	384.46631	-0.1019	2.4412	2.1264	set 7

Table 4. Regression statistics for ozone regression (for UV forecasting)

It can be seen that the regression coefficients vary quite considerably month to month, justifying the monthly updates that are currently being performed.

To test the ozone regression, a predicted ozone value was produced for each NESDIS field of view and compared to the NESDIS ozone value and the default ozone value. The regression was performed in clear and non-clear fields of view and over all surface types, for the area 15°N — 75°N, 60°W — 60°E. Results are displayed in *table 5*, which compares 2 sets of coefficients for November 93 (set 6) and December 93 (set 7) tested on an independent 24 hour period of GLOSS data for 19/01/94 21Z - 20/01/94 21Z.

Ozone regression testing			
		set 6.	*set 7.*
1	NESDIS ozone mean	313.18	313.18
2	NESDIS ozone stan dev	45.48	45.48
3	Predicted ozone mean	287.25	296.87
4	Predicted ozone stan dev	29.75	38.31
5	Default ozone mean	347.00	347.00
6	Default ozone stan dev	0.00	0.00
7	Predicted - NESDIS ozone mean	-25.93	-16.31
8	Predicted - NESDIS ozone stan dev	30.02	27.49
9	Default - NESDIS ozone mean	33.82	33.82
10	Default - NESDIS ozone stan dev	45.48	45.48
11	Max (predicted - NESDIS) diff	147.04	116.73
12	Max (default - NESDIS) diff	206.00	206.00
13	No. predicted - NESDIS diffs > 30 Du	2324	1695
14	No. default - NESDIS diffs > 30 Du	4048	4048
15	No. NESDIS obs used	5735	5735

Table 5. Ozone regression testing (for UV forecasting)

Note : For rows 11-14, the differences are absolute differences, Default ozone = 347 Du.

The number of predicted - NESDIS ozone differences greater than 30 Dobson units (row 13) is less than the number of default - NESDIS ozone differences greater than 30 Dobson units (row 14) and the predicted - NESDIS mean and standard deviation (rows 7 and 8) are less than the default - NESDIS mean and standard deviation (rows 9 and 10) for both sets of coefficients. It is clear, however, that results for set 7 are better than for set 6. Plots of predicted - NESDIS ozone differences using set 6 coefficients and then set 7 coefficients for the area 15°N — 75°N, 60°W — 60°E are shown in *figures 5a,5b* respectively. Some interesting features are seen in *figure 5b*. There is always an area of large predicted - NESDIS ozone differences over the desert areas (Sahara and Saudi Arabia). NESDIS ozone amounts are calculated using a number of HIRS channels, the main being HIRS-9, a surface sensitive

channel. A problem arises due to low emissivity of sand in desert regions resulting in NESDIS cloud-cleared brightness temperatures lower than expected which in turn are interpreted incorrectly as increased ozone absorption [*Chesters and Neuendorffer*, 1991]. In addition there is an uncertainty in surface temperature at the time of observation (large diurnal variation). Large differences also occur over high ground or ice-covered ground e.g. Greenland.

4.2 COMPARISON OF VALUES WITH CAMBORNE

Figure 6 shows daily mean ozone measurements using a Dobson instrument at Camborne (50.2°N, 5.3°W) for the month of September 1993, together with NESDIS ozone and ozone values calculated from equation 2 using regression set 3, plotted as a function of time. The NESDIS ozone amount shows a similar trend to the Camborne measurements throughout the month. On certain days, however, notably on the 9th and the 14th, there are quite large differences.

There are difficulties in estimating NESDIS ozone for a specific area. Whereas the Camborne measurements are daily mean values, the NESDIS ozone amounts are interpolated subjectively from satellite fields of view around the area of interest. Problems occur when data is sparse, either due to general data gaps or to the fields of view being cloudy, or when satellite orbits overlap, when diurnal differences become apparent, with concentrated yet differing ozone values.

The regressed ozone compares to the Camborne amount, with a mean error of 11.5 and a root mean square error of 24.7. The regressed values do not of course show the full variability of the ozone as measured at Camborne or derived by NESDIS, but the general trend of the time function is well predicted, especially in the latter half of the month, where the day to day variation is quite marked.

5. CONCLUSIONS

The predicted ozone values described in section 3 for GLOSS purposes are a useful improvement on using the default value of 347 Dobson units. The replacement of any missing NESDIS ozone values is performed in both clear and non-clear fields of view, but an accurate replacement is only essential for clear fields of view. Due to seasonal variations, regression statistics are updated operationally each month.

The predicted ozone described in section 4 for UV forecasting, agrees to a satisfactory degree with NESDIS ozone for the area of interest to UV forecasts. Larger than expected differences, however, do occur over the Sahara and Saudi Arabia, although this is a frequently seen characteristic, and is consistent with reduced emissivity of a sandy surface as explained in section 4.1. There is satisfactory agreement between the predicted ozone, the NESDIS ozone, and the ground measured ozone at Camborne. It is vital, however, that the regression coefficients are updated monthly to allow for seasonal variations.

ACKNOWLEDGEMENTS

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FIGURE 1A.

Missing NESDIS ozone for cloudy fields of view

For a day in January 1994

FIGURE 1B.

Missing NESDIS ozone for clear fields of view

For a 2 week period in January 1994

FIGURE 2a.

NESDIS ozone in Dobson units

For 20/01/94

FIGURE 2b.

NESDIS ozone in Dobson units

For 20/07/93

FIGURE 3A.

Regressed - NESDIS ozone in Dobson units

Regression for GLOSS using coeff set 6.

For 20/01/94

FIGURE 3B.

Default - NESDIS ozone in Dobson units

For 20/01/94

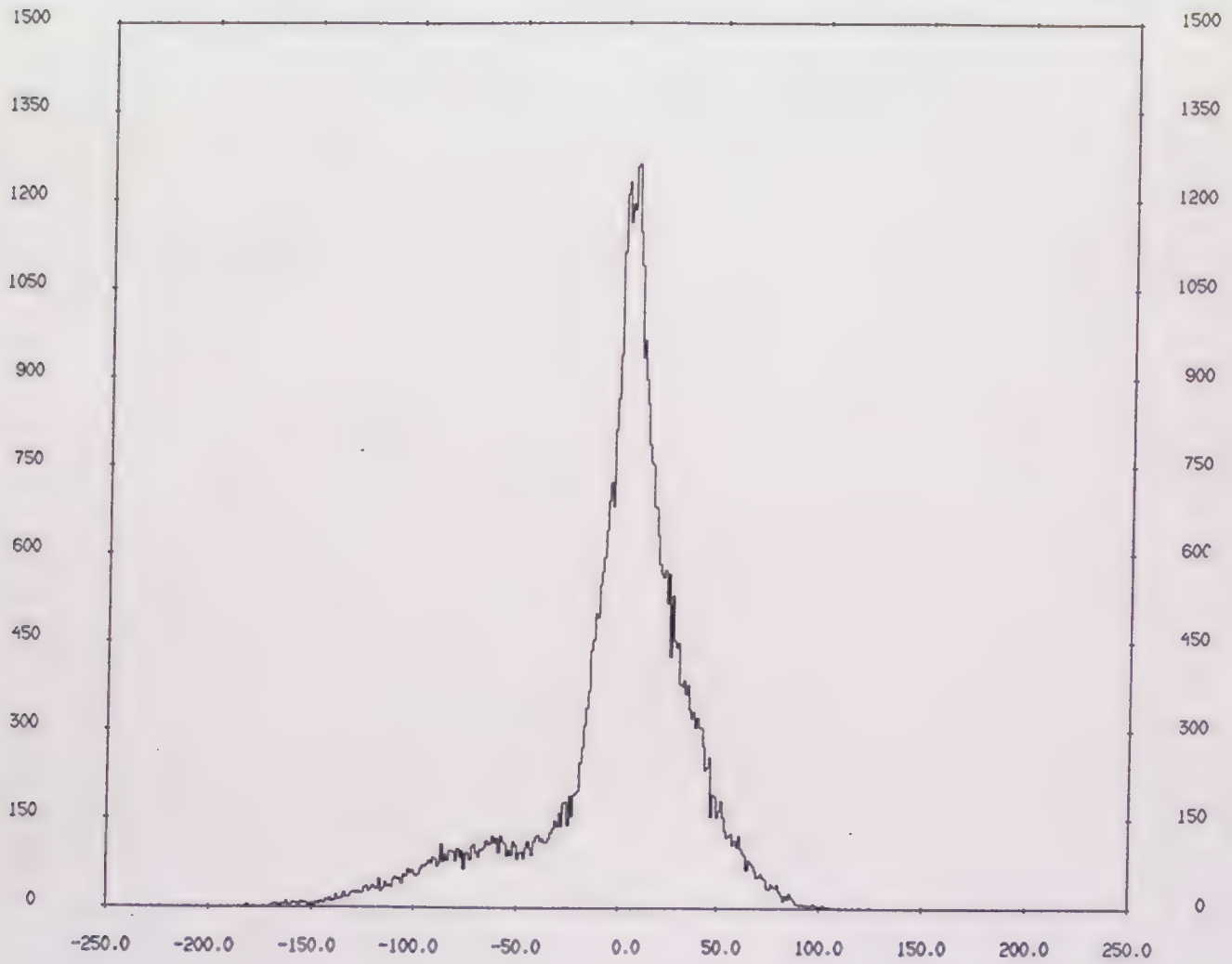

FIGURE 4A.

Regressed - NESDIS ozone in Dobson units

Regression for GLOSS using coeff set 6.

For 20/01/94

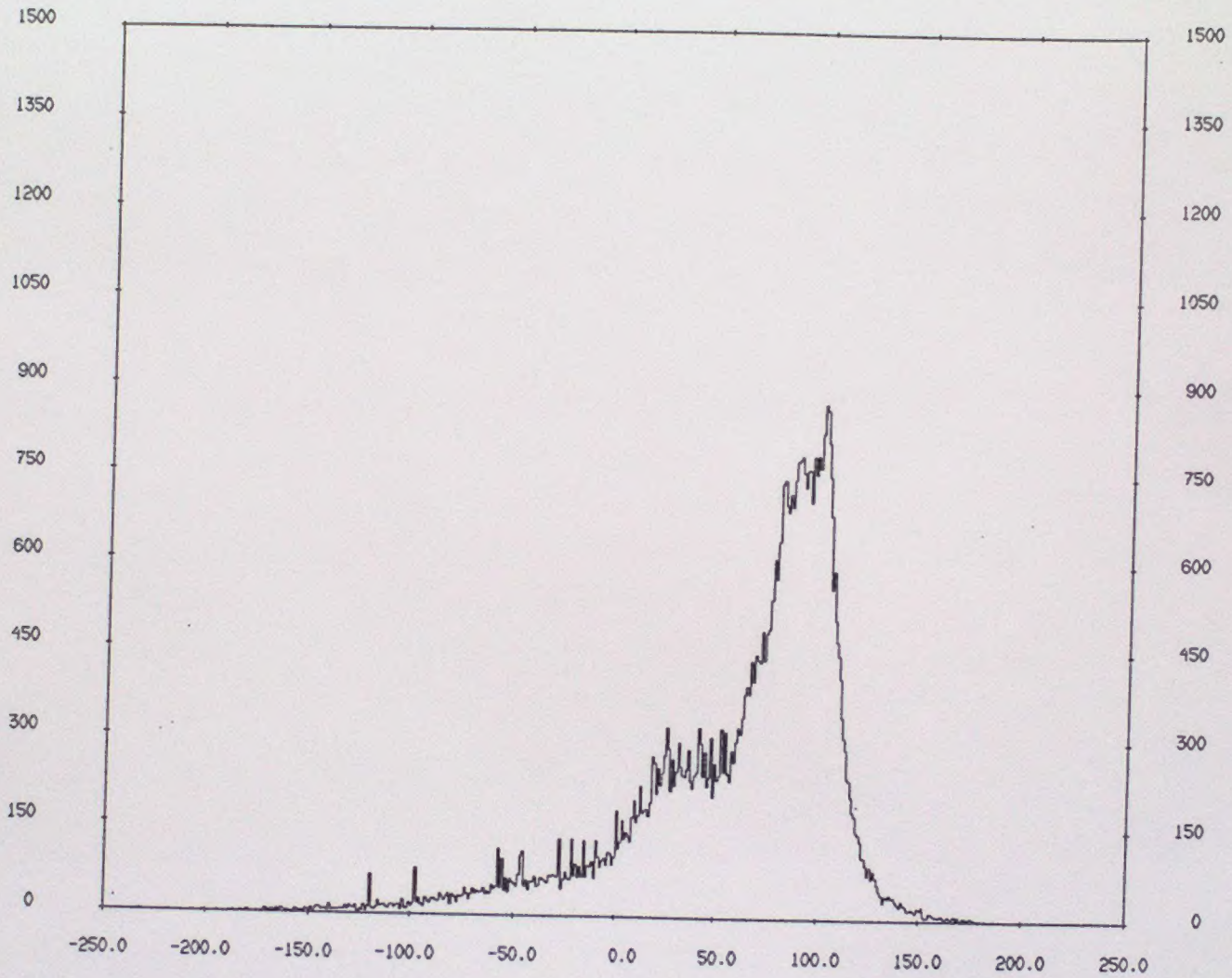

FIGURE 4B.

Default - NESDIS ozone in Dobson units

For 20/01/94

FIGURE 5A.

Regressed - NESDIS ozone in Dobson units

Regression for UV Forecasting using coeff set 6.

For 20/01/94

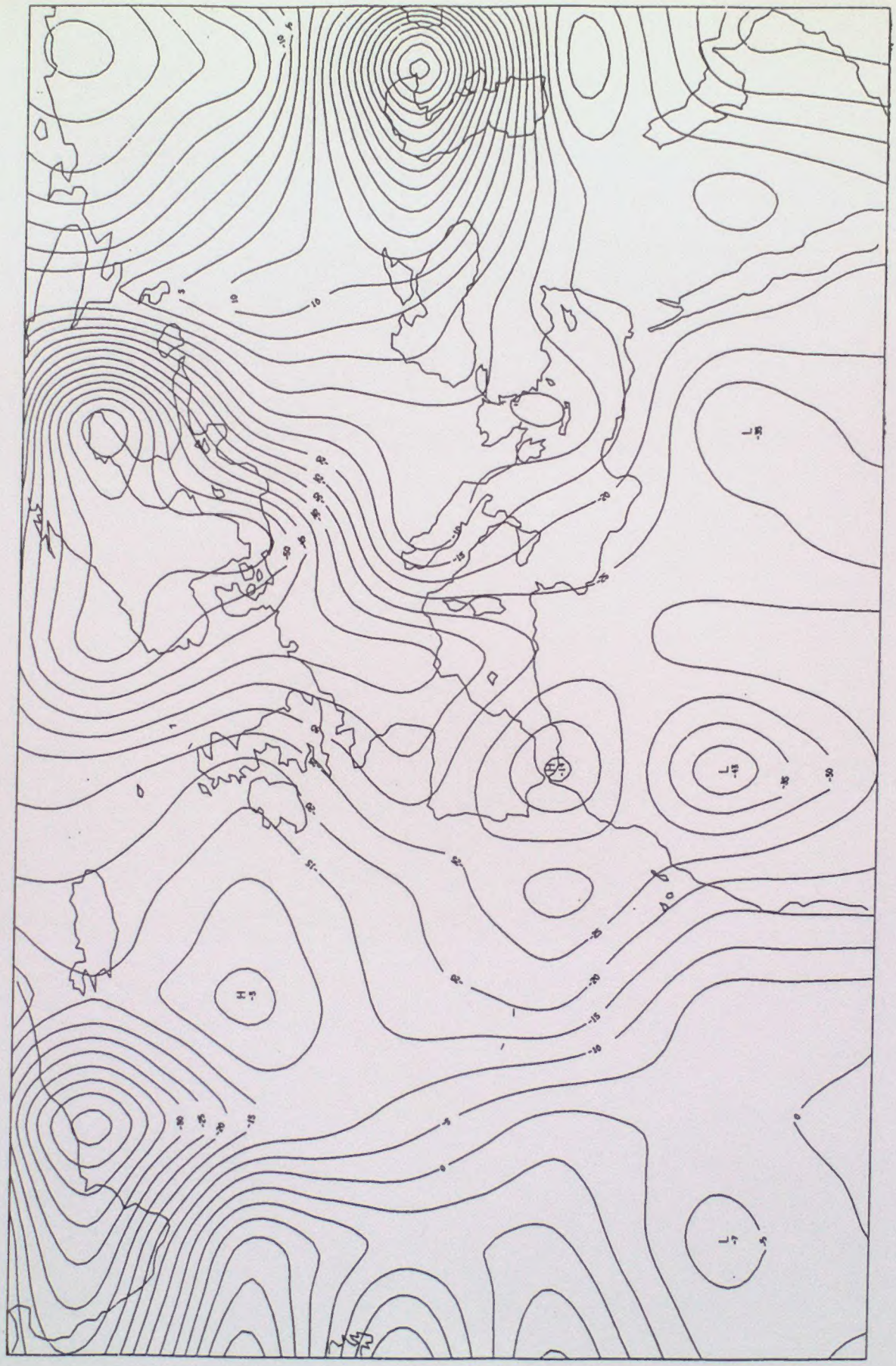

FIGURE 5B.

Regressed - NESDIS ozone in Dobson units

Regression for UV Forecasting using coeff set 7.

For 20/01/94

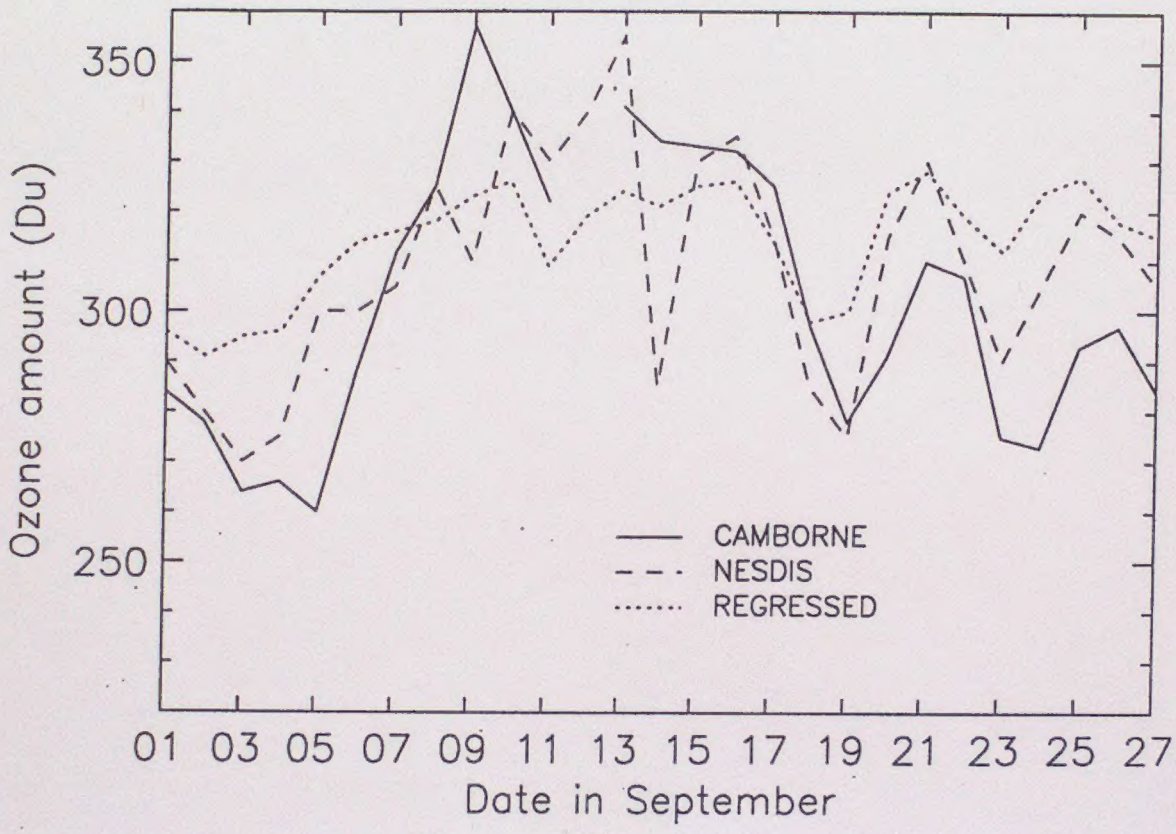

FIGURE 6.

A comparison of regressed ozone with NESDIS ozone and ozone measured at Camborne for September 1993